

# Eigenstate Structure in Graphs and Disordered Lattices

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We study wave function structure for quantum graphs in the chaotic and disordered regime, using measures such as the wave function intensity distribution and the inverse participation ratio. The result is much less ergodicity than expected from random matrix theory, even though the spectral statistics are in agreement with random matrix predictions. Instead, analytical calculations based on short-time semiclassical behavior correctly describe the eigenstate structure.

Quantum graphs, known also as network models, have been used successfully for many years as simple dynamical systems in which to study complex wave behavior. For appropriate parameter values, graphs can be made to display generic chaotic, disordered, or integrable motion, and at the same time the quantum mechanics of these systems has the simplifying advantage of being semiclassically exact. Originally, graphs were developed as models for electrons moving between atoms in an organic molecule [1]. Recently, graph models have been used to study issues as diverse as Anderson localization within the context of periodic orbit theory [2], the spatial distribution and transport properties of persistent currents [3], Aharonov-Bohm conductance modulations in GaAs/GaAlAs networks [4], spectral statistics and the trace formula in chaotic systems [5], spectral determinants, with applications to thermodynamic and transport properties of mesoscopic networks [6], and chaotic scattering and resonance behavior [7]. A discussion of the earlier history of quantum graphs can be found in Ref. [8], which also provides an extensive discussion of the model.

Though substantial work now exists on the spectral and scattering properties of quantum graphs, and also on their large-scale localization behavior, surprisingly little attention has been paid so far to the detailed wave function structure of this paradigmatic quantum system. In this paper we begin to address questions relating to the statistics of wave functions on graphs and their relation to the underlying classical structures in the system. In the process, we examine the relationship between short-time and long-time effects on stationary behavior, making connections to recent work on other simple quantum chaotic problems, including quantum maps, Sinai billiards, Bunimovich stadia, tunneling in double wells, conductance through chaotic quantum dots, and many-body systems with random two-body interactions [9].

A quantum graph consists of  $V$  vertices connected by  $B$  bonds, each of which is modeled as a one-dimensional wire of length  $L_j$  ( $j = 1 \dots B$ ) along which the wave propagates freely with zero potential. At each of the  $i = 1 \dots V$  vertices,  $v_i \geq 2$  bonds will meet (note that  $\sum_i v_i = 2B$ ), and one must impose wave function continuity and the current conservation condition

$$\sum_j \frac{d}{dx} \Psi_{i,j}(x) = \lambda_i \Psi_{i,j}(0), \quad (1)$$

where the sum is over all  $v_i$  bonds  $j$  that meet at vertex  $i$  and  $\Psi_{i,j}(x)$  is the wave function in the bond  $j$ , with  $x = 0$  corresponding to the vertex  $i$ .  $\lambda_i$  is a free parameter associated with the height of the effective potential at vertex  $i$ , and allows one to interpolate between Neumann ( $\lambda_i = 0$ ) and Dirichlet ( $\lambda_i \rightarrow \infty$ ) boundary conditions. One sees easily that the form of Eq. (1) is the only one consistent with an s-wave pointlike scatterer at the vertex; it can be obtained formally using self-adjoint extension theory. Because of time reversal invariance, the wave function in each bond can be written as  $\Psi_{i,j}(x) = a_{i,j}^{(k)} e^{ikx} + a_{i,j}^{(k)*} e^{-ikx}$ , for an eigenstate at energy  $k^2/2m$ . Thus, the distribution of wave function intensities in the system can be completely characterized, in the limit  $kL \rightarrow \infty$ , by the distribution of the quantities  $|a_{i,j}^{(k)}|^2$ . In this limit, the simple normalization condition

$$\sum_{i,j} L_j |a_{i,j}^{(k)}|^2 = \sum_j L_j \quad (2)$$

ensures that the mean bond intensity  $\langle |a_{i,j}^{(k)}|^2 \rangle$  is set to unity.

We begin our analysis with a simple one-dimensional “ring graph” [8] where the  $V$  vertices are arranged in a circle and each vertex  $i$  is connected by bonds to neighboring vertices  $i - v/2 \dots i - 1, i + 1 \dots i + v/2$ .  $v$ , the number of bonds meeting at every vertex, is known as the valency (here taken to be constant over the entire graph). Setting all the vertex potentials  $\lambda_i = 0$  leads to the maximum possible delocalization in the graph (the opposite limit,  $\lambda_i \rightarrow \infty$  would instead produce eigenstates localized on individual bonds), while non-integrability is ensured through randomness in the bond lengths  $L_j$ . In our calculation we take the bond lengths to be uniformly distributed in an interval  $[1 - \delta L, 1 + \delta L]$ ; because the scattering matrices depend only on  $kL_j \bmod 2\pi$ , all choices of  $\delta L$  are equivalent as long as  $\delta L \gg k^{-1}$ . The eigenstates of the system may be obtained by examining a

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$V \times V$  secular matrix  $h(k)$  [8];  $k$  is an eigenvalue whenever  $\det h(k) = 0$ , and the associated null vector corresponds to an eigenvector of the graph. In fact, small but non-zero singular values  $\epsilon$  of  $h(k)$  can easily be seen to correspond to eigenvectors of the same system with slightly perturbed potentials  $\lambda_i \rightarrow \lambda_i - k\epsilon$ , so sufficiently small singular values ( $|\epsilon| < k^{-1}\lambda$ ) can also be used to produce eigenstates. This method allows the collection of several independent wave functions at a given value of  $k$  for any given realization of the disorder ensemble. One easily checks that collecting one or more wave functions at a given value of  $k$  has no discernible effect on the resulting wave function statistics.

Comparing the Heisenberg time ( $\hbar$  divided by the mean level spacing, at which individual levels are resolved) with the time required classically to diffuse over the entire system, or alternatively making an analogy with banded random-matrix behavior, we see that the condition for avoiding localization in our system is  $v^2 \gg V$ . We note that the localization condition is  $k$ - and  $\hbar$ -independent and depends only on the classical graph geometry. Increasing the valency  $v$  for a fixed system size  $V$ , one easily observes a transition from localized to delocalized behavior, which can be detected either by looking at the change in level spacing statistics (from Poisson to GOE) or at the change in the wave function intensity correlation (from strongly negative to near zero) between distant points on the graph. Either method confirms the expected scaling behavior for the transition. One can therefore take the large-volume limit  $V \rightarrow \infty$ , where statistical behavior is expected, while easily satisfying the delocalization condition  $\sqrt{V} < v \leq V - 1$ .

In the delocalized regime, full information about wave function statistical behavior is contained in the distribution of bond intensities  $|a_j^{(k)}|^2$  and their correlations (note that we may freely drop the  $i$  index as it is immaterial which of the two endpoints we take to be the beginning of bond  $j$ ). It is convenient to introduce a simple one-number measure of wave function ergodicity, the inverse participation ratio (IPR):

$$\mathcal{I} = \langle |a_j^{(k)}|^4 \rangle, \quad (3)$$

where the averaging is performed over the  $B = Vv/2$  bonds  $j$  and over a disorder ensemble, at a fixed value of  $k$ . Of course, averaging over nearby values of  $k$  may also be done. It is often useful to introduce a local version of the IPR,  $\mathcal{I}_j$ , where the bond  $j$  is fixed; then  $\mathcal{I} = \langle \mathcal{I}_j \rangle$ , averaging over all bonds. The IPR is the first nontrivial moment of the intensity distribution  $\mathcal{P}(|a_j^{(k)}|^2)$  (we recall that the mean intensity has been normalized to unity), and can range from 1 in the maximally ergodic case where all intensities are equal up to a maximum value of  $B$  in the case of perfect wave function localization on individual bonds. Random matrix theory or the random vector hypothesis would predict Gaussian random fluctuations in the complex coefficients  $a_j^{(k)}$ , thus  $\mathcal{I} = 2$ . An enhancement of the IPR above this baseline value indicates a

deviation from ergodicity in the local wave function behavior.

The key theoretical idea discussed and applied in several recent works [9] is that wave function intensities in a complex system can often be conveniently separated into a product of short-time and long-time parts:

$$|a_j^{(k)}|^2 = \rho_j(E(k)) \times r_{jk}. \quad (4)$$

Here  $\rho_j(E)$  is a smooth local density of states (known alternatively as the strength function) on the bond  $j$  at energy  $E$ , obtained as the Fourier transform of the short-time part of the autocorrelation function

$$A_j^{\text{short}}(t) = \langle j | e^{-iHt} e^{-t/2T_{\text{cutoff}}} | j \rangle, \quad (5)$$

while  $r_{jk}$  is obtained (formally) by Fourier transforming the long-time behavior, at times  $t \sim T_{\text{cutoff}}$  and larger. The decomposition is useful because in many situations the short-time return amplitude  $A_j^{\text{short}}(t)$  has a known approximate analytical expression, which can be transformed to obtain  $\rho_j(E)$ . On the other hand the long-time return amplitude in a chaotic or disordered system is given by a convolution of the short-time behavior with a sum of exponentially many contributions, and thus  $r_{jk}$  may be regarded as random variable:

$$\begin{aligned} \langle r_{jk} \rangle &= 1 \\ \langle r_{jk} r_{j'k'} \rangle &= 1 + (F - 1) \delta_{jj'} \delta_{kk'}, \end{aligned} \quad (6)$$

where the statistical average is performed over an appropriate ensemble. (If  $r_{jk}$  is the square of a complex Gaussian random variable, then  $F = 2$ .) Because the smooth local spectral density  $\rho_j(E)$  and the fluctuations  $r_{jk}$  are associated with distinct time scales (before and after the mixing time, respectively, in a chaotic system), the two quantities are regarded as statistically independent. Thus, for example, the local IPR can be written as

$$\mathcal{I}_j = \langle \rho_j^2 \rangle \langle r_{jk}^2 \rangle = \langle \rho_j^2 \rangle F, \quad (7)$$

where  $\langle \rho_j^2 \rangle$ , the second moment of the smooth local density function, is proportional to the sum of short-time return probabilities  $|A_j^{\text{short}}(t)|^2$ . This formalism has successfully been used to quantitatively study scars of unstable periodic orbits and related phenomena in billiards, in smooth potential wells, and in many-body interacting systems.

To apply these ideas to the ring graphs, we focus on one (arbitrary) bond  $j$  connecting vertices 1, 2. An initial wave packet launched in this bond moving from 1 towards 2 will have a probability

$$P_{\text{trans}} = v^{-2} \left| 1 + e^{-2i \tan^{-1}(\lambda_2/vk)} \right|^2 \quad (8)$$

of being transmitted into one of the other  $v - 1$  bonds meeting at vertex 2; the remaining part of the wave

packet then gets reflected back into the original bond [8]. To begin with, we set  $\lambda = 0$  at all vertices for simplicity, and find that the reflected probability is  $P_{\text{refl}} = 1 - (v - 1)P_{\text{trans}} = 1 - 4(v - 1)/v^2$ . The process is repeated at vertex 1, and the remaining probability  $P_{\text{refl}}^2$  travels again the path taken by the original wave packet, leading to a nontrivial contribution to the return probability. We may iterate this process until almost all of the initial probability to be in the bond  $j$  has decayed (after  $O(1/v)$  bounces for  $v \gg 1$ ), and find that the sum of return probabilities behaves as

$$\int dt |A(t)|^2 \sim \sum_{t=-\infty}^{\infty} (P_{\text{refl}}^2)^{|t|} = \frac{1 + P_{\text{refl}}^2}{1 - P_{\text{refl}}^2} \quad (9)$$

(note that we always sum return probabilities over both positive and negative times). To leading order in  $v$ , we therefore obtain  $\langle \rho_j^2 \rangle = v/4 - O(1)$  for the short-time factor. Taking into account intermediate-time recurrences (where the wave is transmitted at either vertex into an adjoining bond and is subsequently transmitted back into the bond  $j$ ) cancels the  $O(1)$  term, leading to  $\langle \rho_j^2 \rangle = v/4 + O(v^{-1})$ , and thus

$$\mathcal{I} = \mathcal{I}_j = \frac{v}{4} \left(1 - \frac{b}{V}\right) F + O(v^{-1}). \quad (10)$$

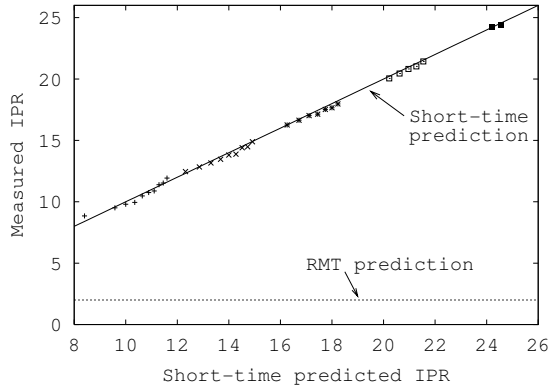


FIG. 1. Observed IPR vs. that predicted by the short-time theory, Eq. (10), for ring graphs with parameter values  $7 \leq v \leq 15$  and  $15 \leq V \leq 33$ . Data points represented by + signs for  $v = 7$ , crosses for  $v = 9$ , stars for  $v = 11$ , empty squares for  $v = 13$  and full squares for  $v = 15$ .

We note that in Eq. (10) we have included the leading  $O(\hbar)$  correction to the semiclassical answer (for graph systems  $V^{-1}$  plays the role of an effective  $\hbar$ , and  $b$  is an undetermined constant). The long-time factor  $F$  can be obtained directly by measuring the mean square value of  $|a_j^{(k)}|^2 / \rho_j(E(k))$ , i.e. of the bond intensity normalized by the analytically computed short-time spectral envelope. For a wide range of values for the system size  $V$  and the valency  $v$ , the result  $4 \leq F \leq 5$  is obtained, supporting the conjecture of independence of short-time and long-time fluctuations in the spectrum (we note  $F > 2$  means

that the long-time fluctuations are super-Gaussian). Numerical data can then be used to fit the coefficient  $b$  of the subleading semiclassical correction; the fit is quite good as can be seen in Fig. 1. As expected, the IPR is primarily a function of valency  $v$ , with volume-dependence being a higher-order effect as long as the delocalization condition  $v^2 > V$  is satisfied. The wave function statistics clearly deviate strongly from random matrix expectations as  $v$  becomes large. This is despite the fact that the level spacing statistics of this system are well-predicted by random matrix theory, indicating an absence of strong localization.

In a one-dimensional system it is of course impossible to take the semiclassical (large-volume) limit for fixed  $v$  while staying in the delocalized regime. It is therefore of interest to consider higher-dimensional systems, such as a  $d$ -dimensional cubic lattice, with  $v = 2d$ . In the absence of vertex potentials ( $\lambda = 0$ ) the above analysis still applies. What happens when we introduce disorder into the system via the potentials  $\lambda_i$  in addition to the disorder already present in the bond lengths? Let the  $\lambda_i$  be independent and distributed for large  $\lambda_i$  in accordance with a power law  $\mathcal{P}(\lambda_i) \sim \lambda_i^{-\alpha}$ , for  $\lambda_0 < \lambda_i < \infty$  (with  $\alpha > 1$ ). We now claim that the tail of the IPR distribution will be strongly modified by the rare events where a strong potential  $\lambda$  is present on both sides of a given bond  $j$  with endpoints 1 and 2. Indeed, we easily see that Eq. (8) for transmission probability reduces to  $P_{\text{trans}} \sim \lambda^{-2}$  for strong  $\lambda$ . Clearly the weaker of the two potentials  $\lambda_1$  and  $\lambda_2$  will dominate the escape rate. The short-time enhancement factor for the local IPR is proportional to the inverse of the escape rate, i.e.  $\mathcal{I}_j \sim \min(\lambda_1^2, \lambda_2^2)$ , and thus we have the prediction

$$\mathcal{P}(\mathcal{I}_j) \sim \lambda_0^{2(\alpha-1)} \mathcal{I}_j^{-\alpha} \quad (11)$$

for  $1 \ll \mathcal{I}_j \ll V$ , modifying the exponential falloff predicted by random matrix theory. Similarly, the tail of the intensity distribution becomes

$$\mathcal{P}(|a|^2) \sim \lambda_0^{2(\alpha-1)} (|a|^2)^{-\alpha-1} \quad (12)$$

for  $1 \ll |a|^2 \ll V$ , in contrast with the exponential Porter-Thomas prediction valid for a system satisfying random matrix statistics.

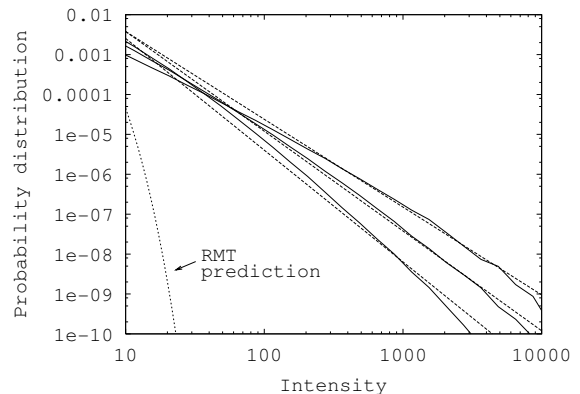


FIG. 2. The tail of the wave function intensity distribution is plotted for a three-dimensional lattice with random potentials  $\lambda$  (see text). From top to bottom, the three solid data curves are for exponent  $\alpha = 1.2, 1.5$ , and  $1.8$ . The corresponding theoretical power laws from Eq. (12) are plotted as dashed lines, with the RMT prediction appearing as a dotted curve for comparison.

The result of Eq. (12) is confirmed in Fig. 2, where we have used an ensemble of  $37^3$  lattices with one out of every  $D = 11$  sites randomly chosen to contain a scatterer (the particle executes free motion while traveling between the scatterer sites, so that the classical motion is diffusive with mean free path  $D$ ). The total number of scatterers is then  $V = 4604$ , and we indeed see that the data curves tend quickly to zero for  $|a|^2 \geq V$ . We have checked that with increasing number of scatterers  $V$  at fixed  $\alpha$ , the intensity distribution curves keep following a given power law behavior for larger and larger intensity, before eventually dropping off to zero. Similarly, we have checked that varying the diffusion constant  $D$  by a factor of 2 does not significantly affect the intensity distribution for fixed  $V$ , as would have been expected for a diffusion-dominated log-normal tail,  $\log \mathcal{P} \sim -D \log^2(|a|^2)$  [10]. We see instead that the tail of the intensity distribution is dominated entirely by the short-time system behavior.

Finally, we return to the volume-averaged IPR  $\mathcal{I}$ , the simplest overall measure of the degree of wave function localization. From Eq. (11), we easily obtain in the large-volume limit

$$\mathcal{I} = C_\alpha \lambda_0^{2(\alpha-1)} V^{2-\alpha}. \quad (13)$$

for  $1 < \alpha < 2$ . As we can see in Table I, this result compares favorably to the numerically computed value over a range of volumes  $V$  and for different classical mean free paths  $D$  and minimum potentials  $\lambda_0$ . None of the IPR's are close to the random matrix prediction  $\mathcal{I} = 2$ .

$V$	$D$	$\lambda_0$	$\mathcal{I}_{\text{predicted}}$	$\mathcal{I}_{\text{actual}}$
549	4	0.3	21	23
549	4	1.0	70	72
2197	8	1.0	141	137
2315	4	1.0	144	131
4604	11	1.0	204	210

TABLE I. Numerically obtained inverse participation ratio  $\mathcal{I}$  for a disordered three-dimensional lattice with exponent  $\alpha = 1.5$ , compared with the prediction of Eq. (13) for various numbers of scatterers  $V$ , mean free paths  $D$ , and minimum potential values  $\lambda_0$ . The constant used is  $C_\alpha = 3.0$ .

In conclusion, we have seen that various aspects of wave function structure in chaotic and disordered quantum graphs are adequately described using the analytically known short-time behavior of the system, specifically the return amplitude at short times and its Fourier transform. On the other hand, random matrix theory completely fails to describe the wave function structure, even though its predictions are good for the spectral statistics. This failure can be understood as resulting from the omnipresence of short periodic orbits in graphs, in contrast with the situation prevailing in most other chaotic systems.

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